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► **To cite this version:**

Wilfried Sigle, Corneliu Sarbu, Dieter Brunner, Manfred Ruhle. Dislocations in plastically deformed SrTiO₃. Philosophical Magazine, 2006, 86 (29-31), pp.4809-4821. 10.1080/14786430600672695 . hal-00513688

HAL Id: hal-00513688

<https://hal.science/hal-00513688>

Submitted on 1 Sep 2010

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Journal:	<i>Philosophical Magazine & Philosophical Magazine Letters</i>
Manuscript ID:	TPHM-05-Dec-0538.R1
Journal Selection:	Philosophical Magazine
Date Submitted by the Author:	01-Mar-2006
Complete List of Authors:	Sigle, Wilfried; Max-Planck-Institut für Metallforschung Sarbu, Corneliu; National Institute for Materials Physics Brunner, Dieter; Max-Planck-Institut für Metallforschung Ruhle, Manfred; Max-Planck Institut, Metallforschung
Keywords:	transmission electron microscopy, brittle-ductile transition, perovskites, plasticity of crystals, dislocation structures
Keywords (user supplied):	



Dislocations in plastically deformed SrTiO₃

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Abstract

Bright-field and weak-beam TEM investigations were performed on plastically deformed SrTiO₃. A gradual change from $a\langle 110 \rangle$ edge-type to screw-type dislocations is found with decreasing temperature. It was found that edge dislocations undergo climb at high temperatures. In order to explain this plastic behaviour a model is presented which is based on the temperature dependence of the dislocation core structures. At elevated temperatures edge dislocations dissociate by climb. This is impeded at low temperatures because of the lack of thermal activation. At low temperatures screw dislocations are assumed to become sessile, probably due to a non-planar dissociation of the dislocation core.

Keywords: Strontium titanate; Plasticity; Dislocation; Brittle-to-ductile transition

1. Introduction

Strontium titanate is an oxide ceramic with perovskite structure. It is cubic except below 105 K where the crystal structure changes to tetragonal and below 65 K to orthorhombic ($c/a = 1.002$). Despite this seemingly simple structure the plastic behaviour (under compression) of this material recently turned out to exhibit quite a spectacular ductile-to-brittle-to-ductile transition (DBDT) [1,2] (see Fig.1).

[Insert Fig.1 about here]

At high temperatures (Regime C) the material yields at stresses which strongly depend on **temperature**. In this temperature regime flow stresses are considerably lower for compression along other directions than $\langle 100 \rangle$ because then the easy glide system $a\langle 100 \rangle\{100\}$ is active [3]. Towards lower temperatures, the material becomes brittle (Regime B), the transition from Regime C to Regime B occurring within a very narrow temperature range. Within Regime B the material fails by brittle fracture at a **temperature**-dependent fracture stress. Most surprisingly, the material becomes ductile again below about 1000 K (Regime A). The flow stress is low (about 150 MPa) and does not vary much until about ambient temperature. At lower temperatures the flow stress increases again. This increase is smooth except around 200 K where the flow stress shows a step-like behaviour (not shown in Fig.1) [4]. Note that this temperature is well above the cubic/tetragonal phase transition and is therefore not related with a structural change of the material.

Notwithstanding the orientation-dependent magnitudes of flow stresses in Regime C there is a general trend of this plastic behaviour irrespective of the crystallographic direction of compression. Slip planes and Burgers vectors were determined by optical polarized light microscopy and transmission electron microscopy (TEM), respectively [3]. For compression along $\langle 100 \rangle$, dislocations with Burgers vector $a\langle 110 \rangle$ (in the following called ' $a\langle 110 \rangle$ dislocations') are predominant in the whole temperature range. For compression along directions different from $\langle 100 \rangle$, $a\langle 110 \rangle$ dislocations are present in Regime A, whereas the slip vector is $a\langle 100 \rangle$ in Regime C.

Because the crystal structure does not change above 105 K it was supposed that this yield behaviour must be related to intrinsic effects of the perovskite material [2]. More precisely, it

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3 was argued that temperature-induced variations of the dislocation core structure might be
4 responsible. In a series of papers we analysed the structures and chemical composition of
5 different dislocation cores: $a\langle 100\rangle\{011\}$ edge [5], $a\langle 110\rangle\{110\}$ edge [6], and $a\langle 100\rangle$ screw
6 [7]. These were dislocations in bi-crystals containing low-angle grain boundaries, i.e. not
7 dislocations formed during plastic deformation. The bi-crystals were diffusion-bonded at 1700
8 K, which is within temperature regime C. It was found that the $a\langle 100\rangle\{011\}$ edge dislocation
9 possesses a compact core structure with a widening of the core of only one lattice constant.
10 On the contrary, the $a\langle 110\rangle\{110\}$ edge dislocation exhibits a climb dissociation into two
11 $a/2\langle 110\rangle$ partial edge dislocations separated by a 2.5 nm wide anti-phase boundary on a
12 $\{110\}$ plane. The $a\langle 100\rangle$ screw dislocation does not show dissociation into separate partial
13 dislocations but detailed analysis of atom positions shows an anisotropic widening of the core
14 along $\langle 110\rangle$ directions. Using electron energy-loss spectroscopy, for all dislocations an
15 increase of the Ti-to-O ratio was found in the core region suggesting a charged core. For the
16 $a\langle 110\rangle\{110\}$ edge dislocation the presence of charge was indeed confirmed by impedance
17 spectroscopy measurements on the same bi-crystals [8].

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19 In the present paper we will present weak-beam and conventional bright-field images of
20 dislocations in single-crystalline specimens deformed within Regimes A and C. These provide
21 new insight into the yield mechanisms.
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2. Experimental

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25 Nominally undoped SrTiO_3 crystals (30 - 200 at.ppm Ca, Ba, and Mg were found by atomic
26 emission spectroscopy) were deformed in compression (for details see [3]). In the present
27 paper we only discuss specimens compressed parallel to the [001] direction. TEM specimens
28 were prepared by ion milling (for details see [3]). The specimens were cut parallel to the
29 principle slip plane (011). The slip planes were selected from light-optical micrographs using
30 polarised light. Since the specimens studied here were compressed along a $\langle 100\rangle$ axis, the
31 crystals were cut at 45° with respect to the compression axis. TEM studies were performed in
32 200 kV microscopes (Philips CM200, JEOL JEM2000FX). Weak-beam images were obtained
33 using (g , $3\dots 4g$) conditions. The analyses involved large tilt angles in order to obtain 3-
34 dimensional information of the dislocation configuration.
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3. Results

3.1 Regime C, 1700 K

The typical dislocation arrangement after deformation in Regime C is shown in Fig. 2 (see also Fig.20 in [3]). It is a view approximately along the [233] axis using $[0\bar{1}1]$ as diffraction vector.

[Insert Fig. 2 about here]

There are predominantly straight edge dislocations from top left to bottom right. In addition, there are curved dislocations (vertical and from bottom left to top right) which have screw components. In Fig. 20 of Ref. [3] also pure screw dislocations were visible in this temperature regime. All dislocations have Burgers vectors of the $a\langle 110 \rangle$ -type, but they belong to different slip systems. This is because under compression along $\langle 100 \rangle$ there exist four equivalent $a\langle 110 \rangle\{110\}$ slip systems of which one is usually dominant because of slight misalignments during compression. The straight dislocations from top left to bottom right have $a[0\bar{1}1]$ Burgers vector and remain straight during tilt around the $[0\bar{1}1]$ axis. A second micrograph of this area is shown in Fig.3.

[Insert Fig. 3 about here]

For this image the crystal was tilted by 52° close to the [001] zone axis using [110] as diffraction vector. This tilt includes a major tilt ($\approx 45^\circ$) around the [100] line direction of the straight edge dislocations. Obviously the dislocation lines appear curved after this tilt. For clarity some corresponding dislocations are marked by letters.

3.2 Regime A, 115 K and RT

Weak-beam dark-field images of dislocation configurations after deformation at room temperature and 115 K are shown in Figs. 4 and 5, respectively.

[Insert Figs. 4, 5 about here]

The diffraction vector \mathbf{g} is $[0\bar{1}1]$. The Burgers vectors of all dislocations are $a[0\bar{1}1]$. Regarding the line directions, after 115 K deformation dislocations are predominantly of

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3 screw type whereas this is much less pronounced for room temperature deformation. Only
4 few pure edge dislocations are visible, some of which are remarkably straight. Most of the
5 dislocations show double contrast. Images taken under $+g$ - and $-g$ -conditions show
6 pronounced inside/outside contrast (Figs.6a,b) indicating that the double contrast is caused by
7 dislocation dipoles.
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11 [Insert Fig. 6a,b about here]
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17 The double contrast is not always continuous along the dislocation line. At some places
18 double contrast is visible at $+g$, whereas at other places $-g$ creates double contrast (marked by
19 white arrows in Fig.6). Despite considerable effort (large tilt experiments) no indication of
20 dislocation dissociation could be found.
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24 Some of the screw dislocations showed a variation of the contrast along their dislocation
25 line (Fig.7), being out of contrast for short segments of the line one of which is marked by an
26 asterisk. The visible parts appeared to be slightly inclined with respect to the general direction
27 of the dislocation line.
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33 [Insert Fig. 7 about here]
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38 4. Discussion 39

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41 Although all types of $a\langle 110 \rangle$ dislocations (from edge to screw) are found in the various
42 temperature regimes, there is a clear trend from edge-type at high temperatures towards
43 screw-type at low temperatures. We therefore believe that the slower moving species are of
44 edge-type at high temperatures and of screw-type at low temperatures.
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50 4.1 Regime C 51

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53 As shown in [3] the dislocations observed in Regime C are $a\langle 110 \rangle$ edge dislocations. These
54 glide on either $(0\bar{1}\bar{1})$, $(1\bar{1}\bar{1})$, or (111) planes. Their straight appearance at small tilt angles
55 (view perpendicular to the slip plane) shows that glide of $a\langle 110 \rangle$ edge dislocations on the
56 (011) slip plane appears to be inhibited. The most likely reason for this is that the dislocations
57 are dissociated by climb. This phenomenon has been frequently observed in oxide ceramics
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3 [9]. For the $a\langle 110 \rangle$ dislocation of concern here, the experimental evidence for dissociation by
4 climb comes from a high-resolution TEM study [6] on bicrystals diffusion-bonded at 1700 K,
5 see Fig. 8. Burgers circuits around the partial dislocations show that their Burgers vectors are
6 $a/2\langle 110 \rangle$. They are arranged vertically above each other. The slip plane of both partial
7 dislocations is horizontal in Fig.8.
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14 [Insert Fig. 8 about here]

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17 The dissociation width is about 2.5 nm which is too narrow to be resolved in Figs.2 and 3.
18 With regard to the elastic energy this type of dissociation is more stable than dissociation on
19 the slip plane. This is displayed in Fig.9 which shows the forces acting between two $a/2\langle 110 \rangle$
20 partials [10]. These are calculated on the basis of anisotropic elasticity theory.
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26 [Insert Fig. 9 about here]

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29 One of the partials is located in the centre ($x = 0, y = 0$) of Fig. 9. The slip plane is horizontal.
30 The arrows show the direction and strength of the force acting on the second partial at the
31 arrow position. The forces acting on the dislocations tend to lead to dissociation on the slip
32 plane if no climb forces are present. However, once one of the partials has undergone climb,
33 the force is directed away from the slip plane. Under these conditions the elastic forces drive
34 the partials into the stable 'climb configuration' where both partials are placed vertically
35 above each other.
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42 One might ask whether dissociation by climb is kinetically possible since climb requires the
43 diffusion of all three atom species, O, Sr, and Ti. Diffusion activation enthalpies in the bulk
44 are 1 eV for oxygen and 3.5—4 eV for Sr [11, 12]. For Ti no reliable data exist, but it is
45 assumed that the diffusion of Ti is the slowest among the three species [12]. It is important to
46 note that for 'climb dissociation' diffusion is required only between the partials (i.e. on the
47 nanometre scale) which means that only few atom jumps are necessary. Furthermore, in the
48 core region of the dislocation diffusion barriers are certainly shallower than in the bulk, i.e.
49 the mentioned activation enthalpies are upper limits. This is probably the reason why Rhodes
50 and Kingery [13] found an activation energy for dislocation pipe diffusion of Ti of only 4.9
51 eV. These numbers indicate that, under the assumption that core diffusion governs the kinetics
52 of the climb process within Regime C, all three species should be able to migrate over
53 distances required to make climb dissociation possible. Therefore we assume that $a\langle 110 \rangle$
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3 edge dislocations are dissociated by climb over their whole length within Regime C (Fig.
4 10b).

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7 Fig. 3 was obtained after a large-angle tilt with the projection of the straight edge
8 dislocations as tilt axis. Their curvature shows that the dislocations have moved in a plane
9 different from their slip plane (Fig.10c).

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14 [Figure 10 about here]

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17 This means that they have undergone climb. The straight appearance of the dislocations when
18 observed perpendicular to the glide plane (Fig. 2) shows that glide appears to be inhibited,
19 most likely because of the possible 'climb dissociation' mentioned above. For glide the
20 partials would have to recombine, thus removing the APB between them, or the APB would
21 have to be dragged along with the partials which would lead to the formation of small
22 dislocation loops. Such loops were indeed observed (see Fig.22 in Ref. [3]) but only very
23 sparsely in some of the TEM samples. In most areas, like those shown in Figs.2 and 3, such
24 structures are not present. Therefore we assume that the dissociated dislocation remains in its
25 elastically stable climb-dissociated configuration and as such undergoes climb.

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Macroscopic deformation governed by this climb process needs considerable thermal
activation because long-range diffusion of all three atom species, Ti, O, and Sr is required.
The large activation enthalpies for cation migration (at least 3.5 eV for Sr and even more for
Ti [11, 12]) make strong thermal activation necessary for cation diffusion to take place. This
is reflected in the strong temperature dependence of the flow stress within Regime C.
According to Taeri et al. [3] the activation energy for dislocation movement in Regime C is
about 6 eV for compression along $\langle 100 \rangle$. This is higher than the activation enthalpy for
diffusion of Sr and O, but it might be of a similar magnitude as the Ti diffusion enthalpy. It
should be mentioned that extremely high diffusion enthalpies for Ti were reported (>10 eV)
[14] which would be way too high to make Ti diffusion possible within Regime C. However,
Gömann et al. [15] found evidence for Ti migration via Sr vacancies, and Sr vacancies are
much easier to form than Ti vacancies. Ti diffusion via Sr vacancies would, however, lead to
some chemical disorder in the wake of the climbed dislocation. How this would influence the
dislocation mobility is not clear presently.

Wang et al. [16] performed extensive creep studies of $\langle 100 \rangle$ - and $\langle 110 \rangle$ -oriented SrTiO₃
single crystals. They found similar dislocation arrangements as presented in this paper. From
the straight appearance of $a\langle 110 \rangle$ edge dislocations when observed perpendicular to the slip

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3 plane they concluded that these dislocations move by glide. The present study shows that this
4 interpretation is erroneous.
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7 8 9 **4.2 Regime B**

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11 Within Regime B specimens fracture at a fracture stress which strongly increases as
12 temperature increases. The material shatters into small pieces indicating that cracks nucleate
13 in the interior of the material. The formation of such cracks requires high internal stresses. To
14 explain this we assume that the climb dissociation described above also occurs within Regime
15 B, however, because of the lower temperature, only locally along short dislocation segments
16 (Fig. 10a). Unlike in Regime C, these short segments are sessile in Regime B, i.e. only the
17 glissile segments in between are able to move by bowing out under the applied stress (Fig.11).
18 The movement of these glissile segments will soon be retarded by the formation of new
19 sessile segments. This means that long-range motion of dislocations is not possible in Regime
20 B which is reflected in the absence of plastic yielding. A further consequence is that
21 dislocations will not be able to move long distances from the dislocation sources, thus
22 forming obstacles for dislocations emitted from the same source later on. We suppose that the
23 resulting pile-ups lead to sufficiently high internal stresses to initiate crack formation.
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37 [Figure 11 about here]
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41 Increasing temperature leads to shorter mobile segments for which the Orowan stress, which
42 is required for movement, becomes higher. This would explain the increasing fracture stress
43 with increasing temperature. Presently it is unclear how the high internal stresses develop. A
44 possible mechanism would be the pile-up of dislocation loops emanating from the mobile
45 dislocation segments, at obstacles. The dislocation configuration within Regime B is very
46 complicated, showing isolated bundles of dislocations of various Burgers vectors (see Ref.
47 [3]).
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60 **4.3 Regime A**

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3 At the high-temperature end of Regime A edge dislocations dominate, as it is the case in
4 Regime C. This might be related to the beginning formation of sessile dislocation segments on
5 the edge components disabling the edge segments from changing their line orientation.
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7 However, at lower temperatures this will not be possible any more because of the lack of
8 thermal activation. Therefore the dislocations remain on their slip plane and dislocation
9 dissociation is possible only on this plane. As shown in Fig. 4, room temperature deformation
10 leads to the formation of dislocations of various types and deformation at 115 K results
11 predominantly in screw-type dislocations. For this reason it is likely that towards low
12 temperatures plasticity is governed by screw dislocations. The increase of the flow stress
13 towards lower temperatures and the abundance of screw dislocations can then be interpreted
14 as a decrease of the screw dislocation mobility. Within the Peierls model this could be
15 explained by a high Peierls potential which may originate simply from the strong (partially
16 ionic) bonds in SrTiO₃ or from the particular core structure of screw dislocations. The latter
17 would resemble the situation in bcc metals where the core of $a\langle 111 \rangle$ screw dislocations
18 dissociates in a non-planar threefold manner which makes thermal activation necessary to
19 make the dislocation mobile. In the case of the $a[0\bar{1}1]$ screw dislocation in SrTiO₃ the core
20 symmetry is two-fold according to the crystal symmetry. The possible low-index dissociation
21 planes are (100), (011), (111), and $(\bar{1}11)$. Especially for the case of a dissociation on the two
22 {111} planes a sessile non-planar configuration of the core could be envisaged. Maybe it is
23 worth noting that we indeed observed a non-planar core configuration of the $a\langle 100 \rangle$ screw
24 dislocation in SrTiO₃ using HRTEM [7]. We found that the displacement field is more
25 pronounced along $\langle 110 \rangle$ directions than along $\langle 100 \rangle$ directions. A similar study for $a\langle 110 \rangle$
26 dislocations remains to be done.
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45 The observed screw-type dislocations occur as dislocation dipoles. Apparently the dipole
46 configuration is rather stable. At sites marked by white arrows in Fig.6 the dipoles change
47 between two stable configurations. This leads to the variation of the inside/outside contrast
48 along the dislocation line. The partially vanishing contrast of the screw dipoles is probably
49 due to the local constriction of the two screws, leading to the annihilation of the dipole. For
50 screw dipoles this should be easily achievable if glide on the plane connecting the two
51 dislocations is possible. This connecting plane is the (100) plane in Fig.6. After the
52 constriction elongated dislocation loops are left behind which have short edge components at
53 their two ends. The partial bending or even rotation of the loops indicates that their
54 energetically preferred plane is not the (100) plane.
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3 Unfortunately dissociation of dislocations by glide could not be observed until now
4 although this should be quite likely for dislocations with such a long Burgers vector. This
5 indicates that the APB energy on the possible slip planes is pretty high. Matsunaga and Saka
6 [17] reported on dissociation of $a\langle 110 \rangle$ dislocations formed by indentation at room
7 temperature. The double contrast they observe is similar to that found in our investigations.
8 However, they did not perform $+g/-g$ -experiments. Our $+g/-g$ -experiments clearly show that
9 the double contrast is due to dislocation dipoles and not to dissociation.
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20 5. Conclusion

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22 We have performed extensive TEM studies of SrTiO₃ single crystals plastically deformed by
23 compression along the $\langle 100 \rangle$ direction. The main results are:

- 24
25 (i) In the temperature range from 100 K to 1000 K we found almost exclusively dislocations
26 with Burgers vector $a\langle 110 \rangle$. However, there is a clear tendency from screw-type to edge-type
27 as temperature increases. The straight appearance of screw dislocations at low temperatures
28 indicates low mobility the reason of which remains speculative at present. We assume that the
29 particular core structure of these dislocations makes them sessile as temperature decreases.
30 This might be possible to be revealed by high-resolution TEM, in a similar way as was done
31 for the bcc metal Mo [18].
32
33 (ii) We have shown clear evidence for dislocation climb at high temperatures. The possibility
34 of this process is supported by the similar magnitude of the activation enthalpies for
35 dislocation motion and of cation diffusion.
36
37 (iii) A model, based on the climb dissociation of $a\langle 110 \rangle$ edge dislocations, was proposed to
38 explain the pronounced DBDT of this perovskite material.
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49 It is still puzzling why dissociation of dislocations in Regime A could not be observed up to
50 now by the weak-beam method. The dissociation width must be below 2 nm indicating a high
51 APB energy on the $\{110\}$ plane. The knowledge of planar-fault energies γ (the ' γ surface') in
52 SrTiO₃ is clearly required in order to gain further insight into the dissociation mechanisms.
53 Hopefully this can be achieved soon by the help of *ab initio* calculations.
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Acknowledgements

We are indebted to U. Salzberger and M. Sycha for the excellent TEM specimen preparation. Discussions with Prof. V. Vitek and A. Heuer are gratefully acknowledged. We thank the German Science Foundation for financial support of C.S. in the framework of the Research Training Group GRK 285. We thank the Referees for very helpful comments which allowed us to improve the paper.

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References

- [1] D. Brunner, S. Taeri-Baghadrani, W. Sigle, M. Rühle, *J. Am. Ceram. Soc.* **84** 1161 (2001).
- [2] P. Gumbsch, S. Taeri-Baghadrani, D. Brunner, W. Sigle, M. Rühle, *Phys. Rev. Lett.* **87** 085505 (2001).
- [3] S. Taeri, D. Brunner, W. Sigle, M. Rühle, *Z. Metallkd.* **95** 433 (2004)
- [4] D. Brunner, private communication
- [5] Z. Zhang, W. Sigle, M. Rühle, *Phys. Rev.* **B66** 094108 (2002)
- [6] Z. Zhang, W. Sigle, W. Kurtz, M. Rühle, *Phys. Rev.* **B66** 214112 (2002)
- [7] Z. Zhang, W. Sigle, W. Kurtz, *Phys. Rev.* **B69** 144103 (2004)
- [8] R. A. de Souza, J. Fleig, J. Maier, O. Kienzle, Z.L. Zhang, W. Sigle, M. Rühle *J. Am. Ceram. Soc.* **86**, No.6, 922 (2003)
- [9] T.E. Mitchell, K.P.D. Lagerlöf, A.H. Heuer, *Mater. Sci. Techn.* **1** 944 (1985)
- [10] Calculated by a computer code written by Prof. V. Vitek.
- [11] R. Meyer, R. Waser, J. Helmbold, G. Borchardt, *Phys. Rev. Lett.* **90** 105901 (2003)
- [12] K. Gömann, G. Borchardt, M. Schulz, A. Gömann, W. Maus-Friedrichs, B. Lesage, O. Kaïtasov, S. Hoffmann-Eifert, T. Schneller, *Phys. Chem. Chem. Phys.* **7** 2053 (2005)
- [13] W.H. Rhodes, W.D. Kingery, *J. Am. Ceram. Soc.* **49** 521 (1966)
- [14] M.J. Akhtar, Z. Akhtar, R.A. Jackson, *J. Am. Ceram. Soc.* **78** 421 (1995)
- [15] K. Gömann, G. Borchardt, A. Gunhold, W. Maus-Friedrichs, H. Baumann, *Phys. Chem. Chem. Phys.* **6** 3639 (2004).
- [16] Z. Wang, S.-I. Karato, K. Fujino, *Phys. Earth Planet. Inter.* **79** 299 (1993).
- [17] T. Matsunaga, H. Saka, *Phil. Mag. Lett.* **80** 597 (2000).
- [18] W. Sigle, *Phil. Mag.* **79** 1009 (1999).

Figure captions

Fig.1: Temperature dependence of the flow stress, τ_o , and fracture stress, τ_{fr} , in SrTiO₃ under compressive loading along different crystallographic axes. Three different regimes can be distinguished: Regime A at low temperatures where the flow stress is low but increasing towards low temperatures, Regime B where the material fails catastrophically at a temperature-dependent fracture stress, and Regime C where a strongly temperature-dependent flow stress is found. The classification labels (A, B, C) shown in the upper part of the Figure are for the $\langle 100 \rangle$ compression axis, whereas those shown in the lower part (a, b, c) are for orientations other than $\langle 110 \rangle$. The low-temperature flow stresses coincide for all orientations, but the temperature range of Regime B and the high-temperature flow stresses are orientation-dependent. This is related with the different glide systems: The easy glide system $a\langle 100 \rangle\{100\}$ which is active for non- $\langle 100 \rangle$ compression in Regime C cannot operate with a load parallel to $\langle 100 \rangle$ because of the vanishing Schmid factor.

Fig.2: Bright-field image of the dislocation configuration after deformation in Regime C. The incident beam direction is close to $[233]$. Most of the observed dislocations are straight, running from top left to bottom right, and are of edge type with Burgers vector $a[01\bar{1}]$. The other dislocations (vertical line direction and from top right to bottom left) also have $a\langle 110 \rangle$ Burgers vectors but are no pure edge dislocations (for details see Reference [3]). They belong to other $a\langle 110 \rangle\{110\}$ slip systems which are all activated by compression along $\langle 100 \rangle$.

Fig.3: Bright-field image of the same area as Fig.1 but tilted by 52° . The observation direction is close to $[001]$. The straight dislocations in Fig. 1 are now clearly curved. For clarity some corresponding dislocations are marked by letters. The double contrast of dislocations marked by asterisks is because $g \cdot b$ is equal to 2 whereas the product is unity for the other dislocations.

Fig.4: Weak-beam image of the dislocation configuration after deformation at room temperature. The dislocations have various line directions with a slight bias towards the screw orientation (parallel to g).

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5 Fig.5: Weak-beam image of the dislocation configuration after deformation at 115 K. Unlike
6 the dislocation pattern at room temperature, here dislocations are mostly of pure screw type
7 and few of them of pure edge type.
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12 Fig.6: Weak-beam images taken under $+g$ - and $-g$ -conditions showing pronounced
13 inside/outside contrast. The image is an enlarged part of Fig. 5. The double contrast is not
14 always continuous along the dislocation line. At some places double contrast is visible at $+g$,
15 whereas at other places $-g$ creates double contrast (marked by arrows).
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21 Fig.7: Weak-beam image of screw dislocations showing a variation of the contrast along their
22 dislocation line. **One location where the contrast has vanished is marked by an asterisk.** The
23 dipoles appear to be decomposed into dislocation loops. The loops appear to be slightly
24 inclined with respect to the general direction of the dislocation line. The image is an enlarged
25 part of Fig. 5.
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32 Fig.8: HRTEM image of an $a\langle 110 \rangle$ edge dislocations dissociated by climb. This image is
33 taken from a bicrystal specimen containing a low-angle $\langle 110 \rangle$ tilt grain boundary [6].
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37 Fig.9: Plot of the forces acting between two $a/2\langle 110 \rangle$ partials. One of the partials is in the
38 centre ($x = 0, y = 0$). The slip plane is horizontal. The arrows show the direction and strength
39 of the force acting on the second partial at the arrow position.
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44 Fig.10: Sketch of the possible structure of the $a\langle 110 \rangle$ edge dislocation in Regimes B and C.
45 Two adjacent $\{110\}$ planes are shown in grey. The non-dissociated dislocation is located on
46 the upper plane. (a) The dislocation is dissociated by climb along a short segment. (b) The
47 dislocation is dissociated along its whole length. (c) The dislocation has moved out of the slip
48 plane by climb, **i.e. perpendicular to the slip plane.**
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54 Fig.11: Sketch of the $a\langle 110 \rangle$ edge dislocation being dissociated on the left and right side.
55 The non-dissociated part can bow out under an applied stress.
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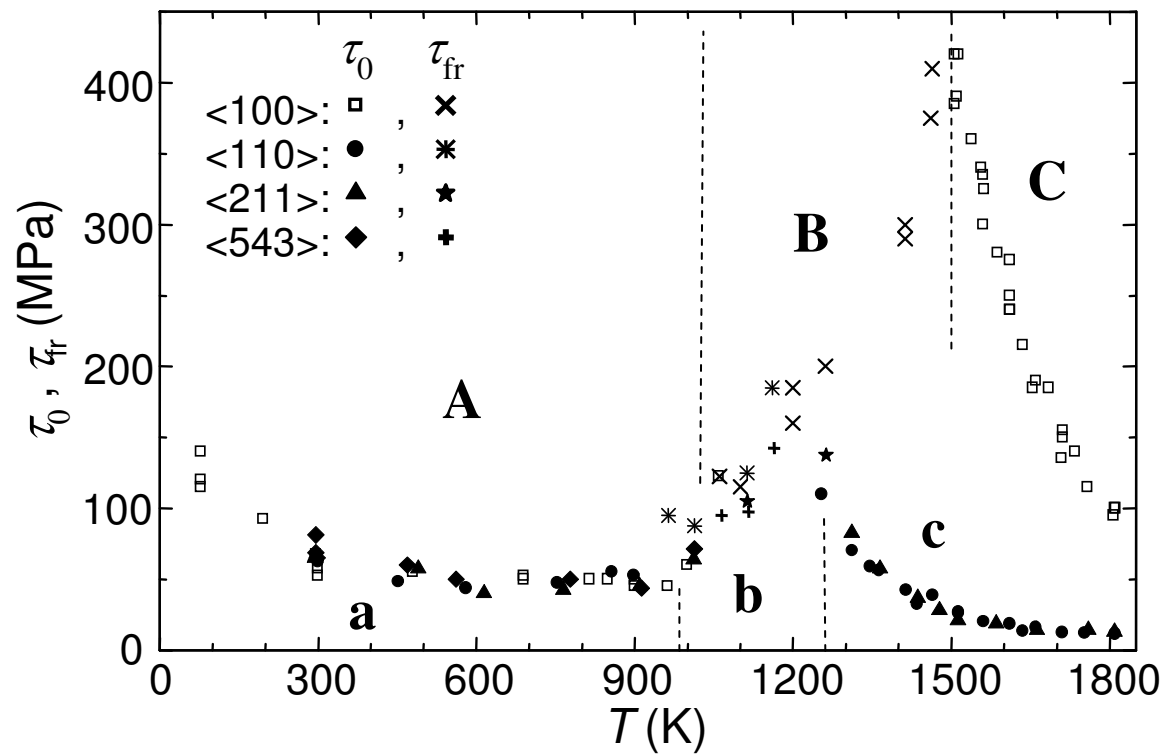


Fig. 1

Fig.2

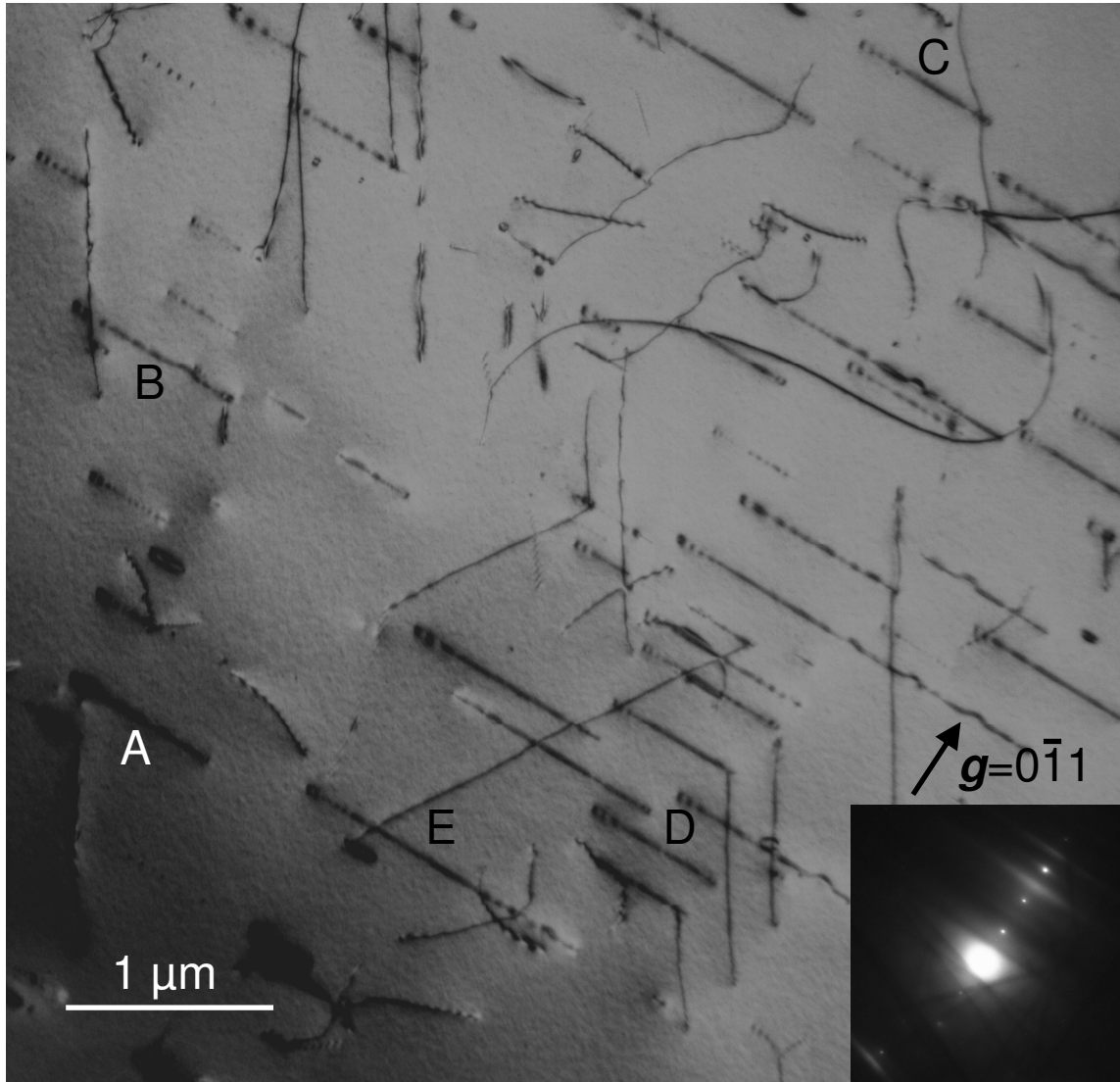


Fig.3

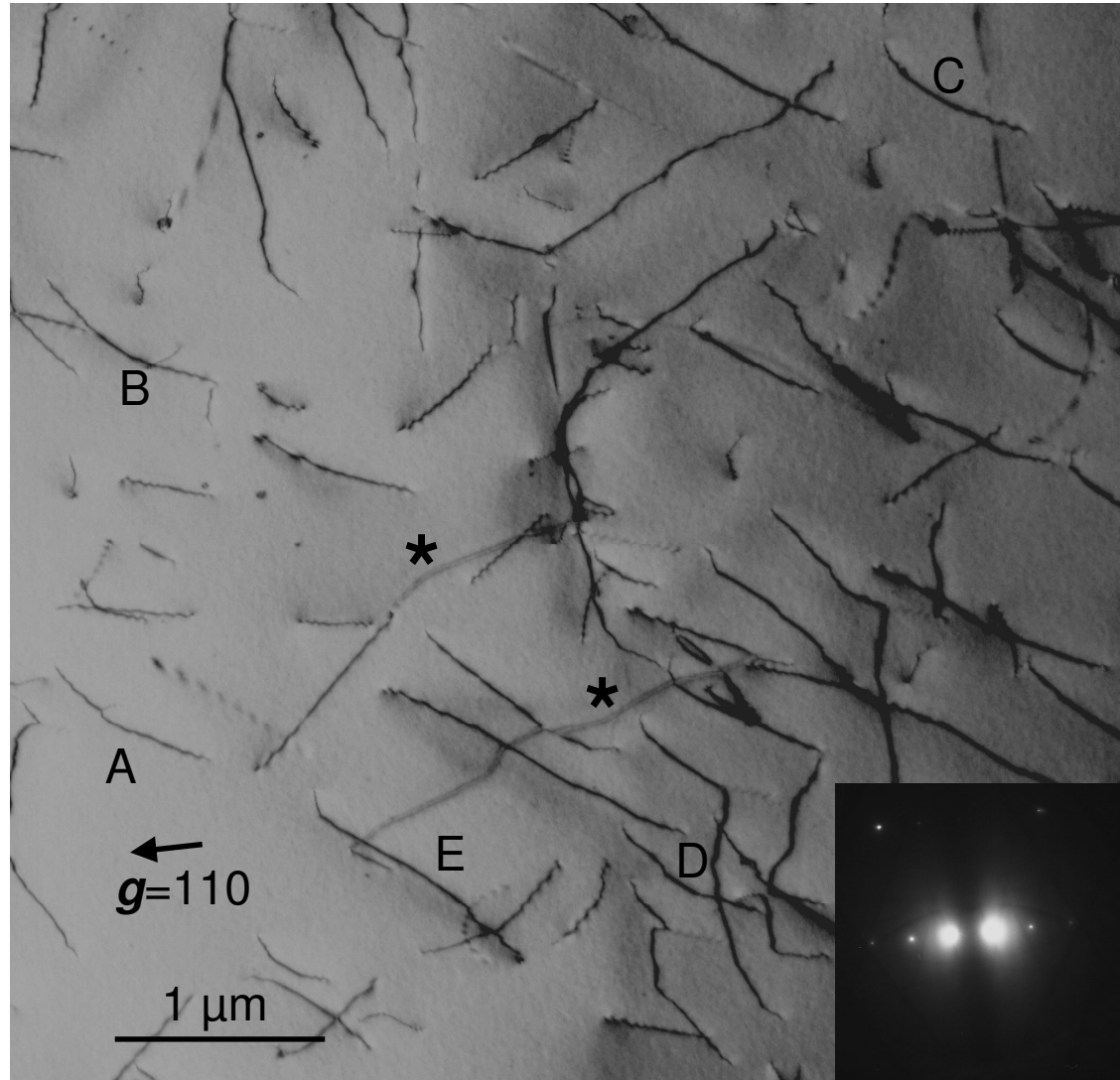
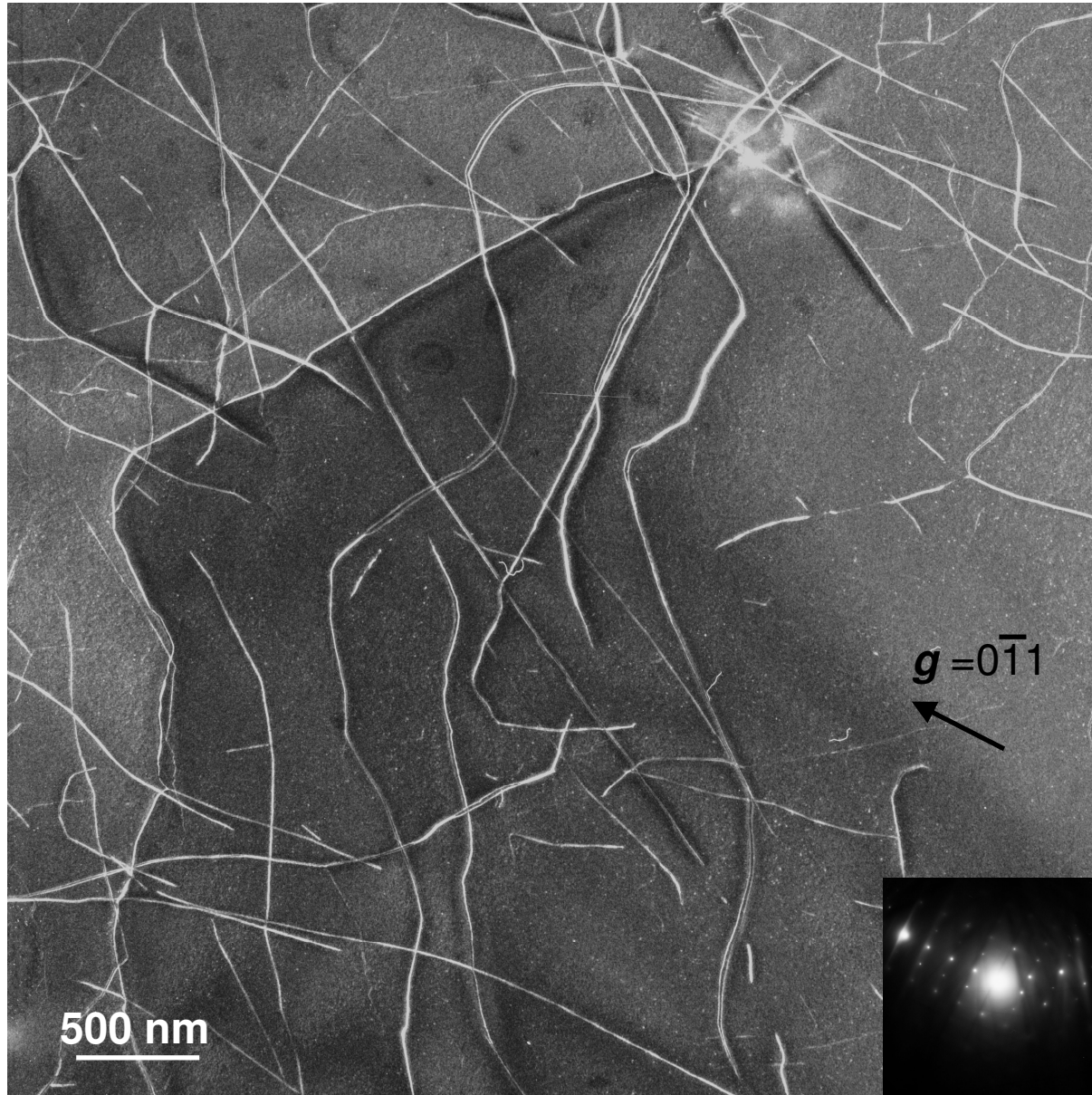


Fig. 4



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Fig.5

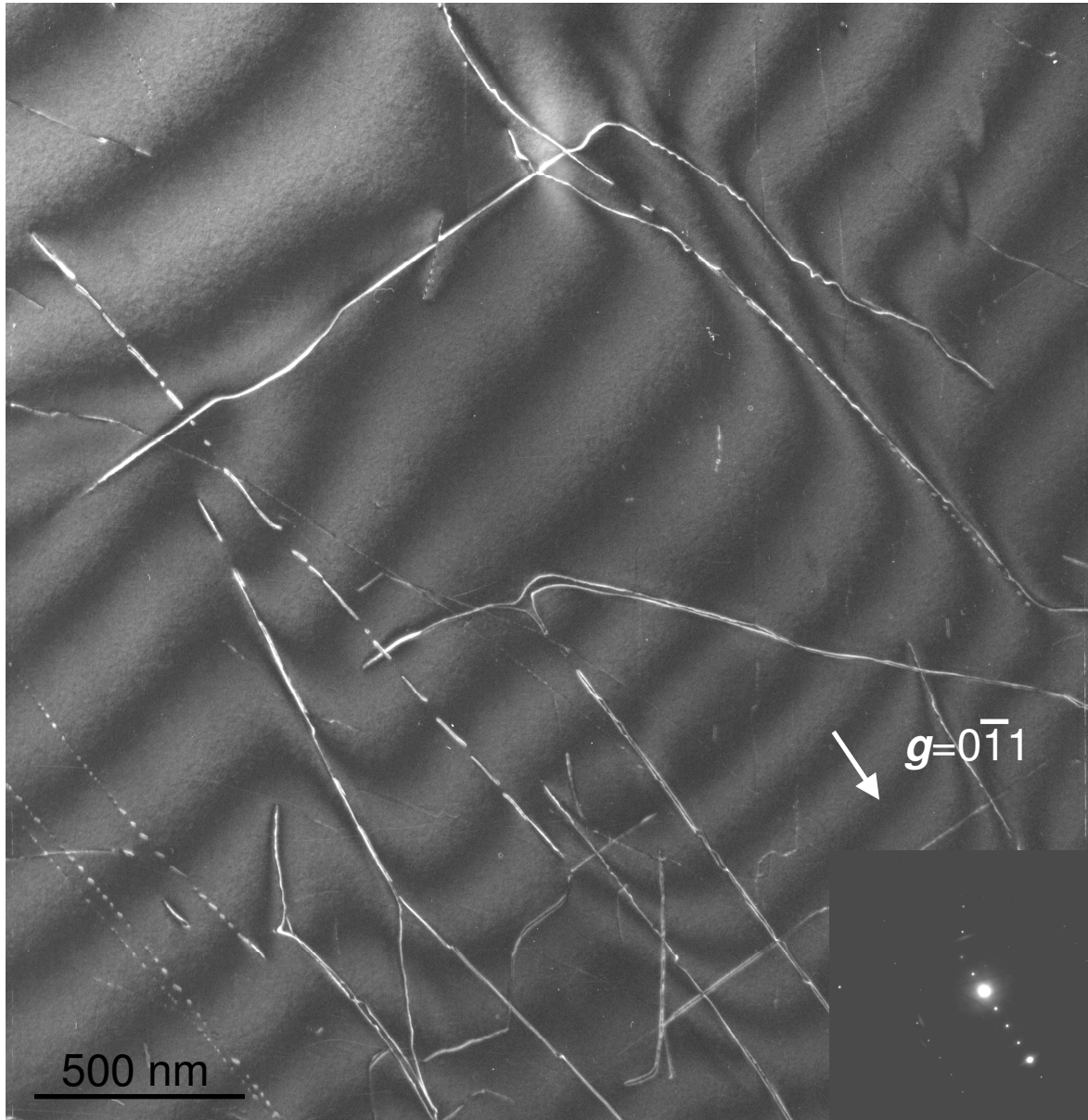


Fig.6

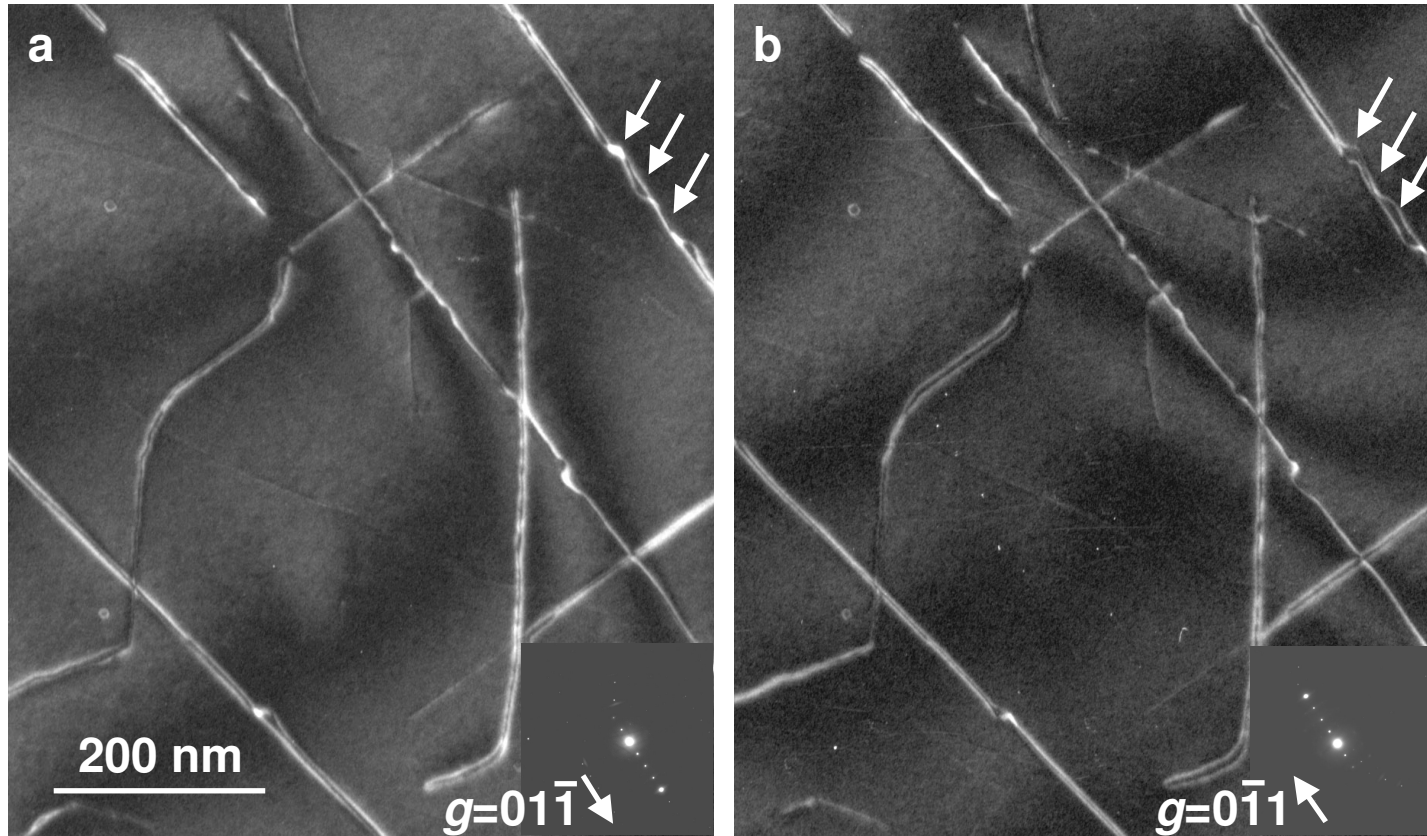


Fig.7

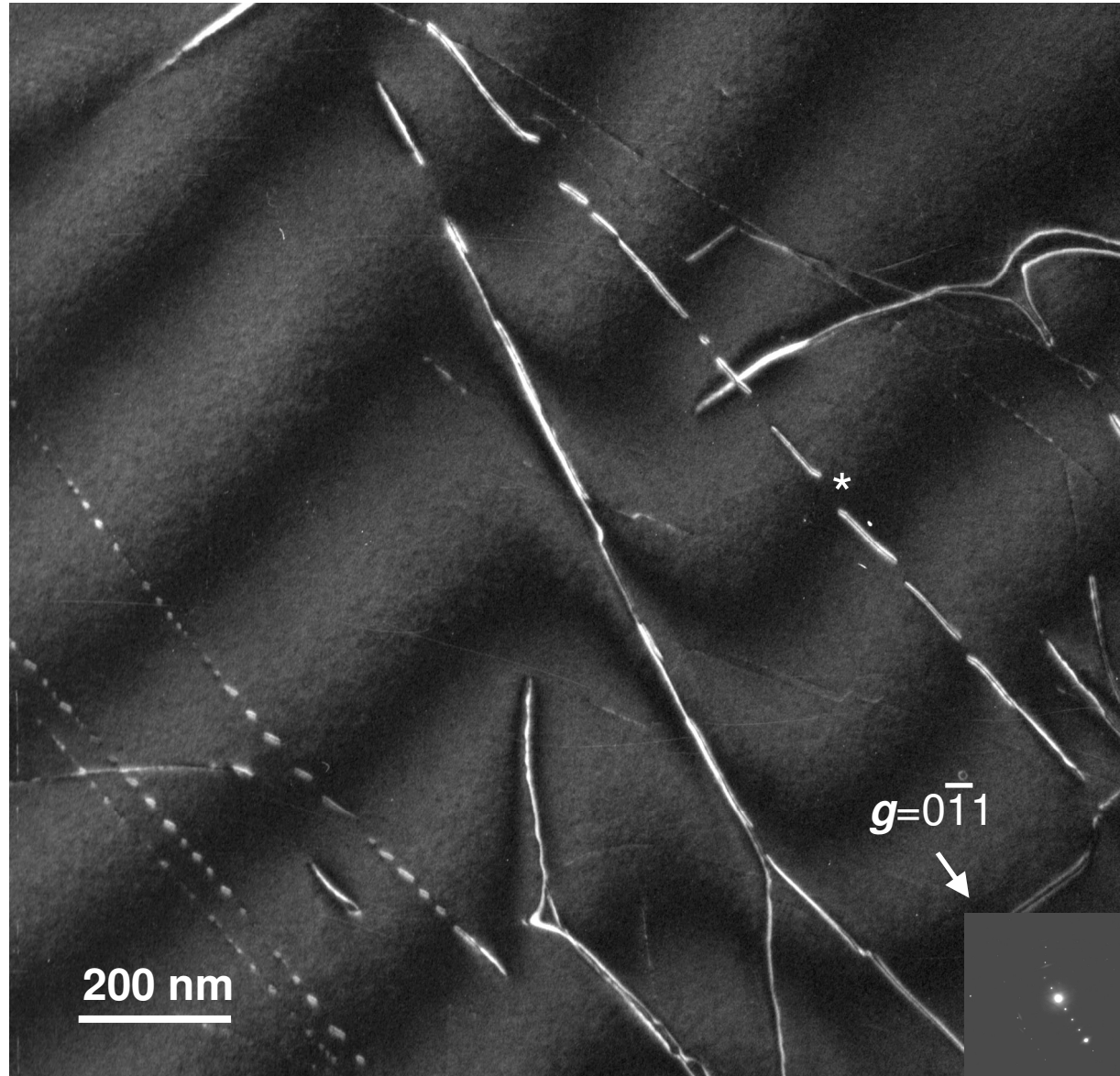


Fig.8

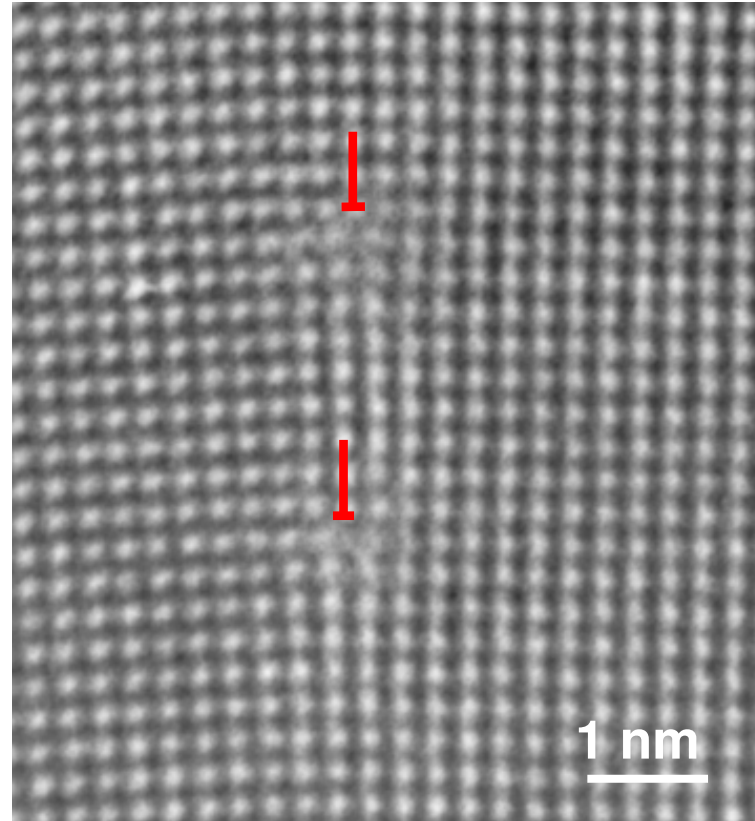
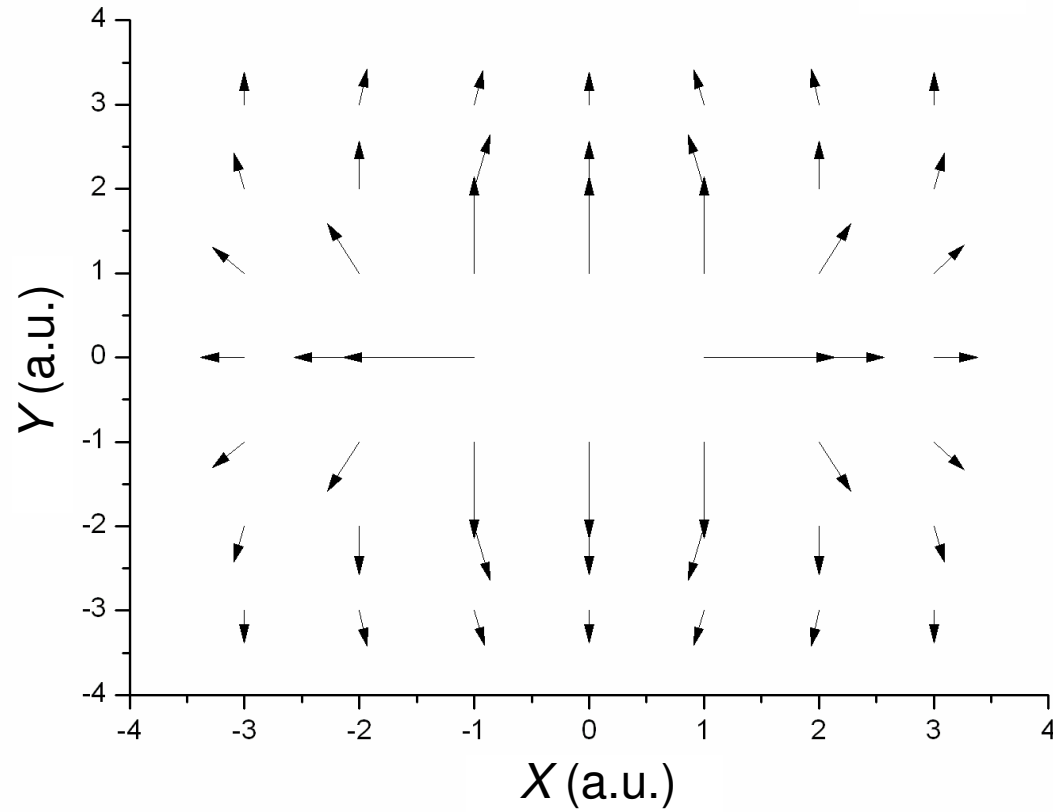


Fig.9



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Fig.10

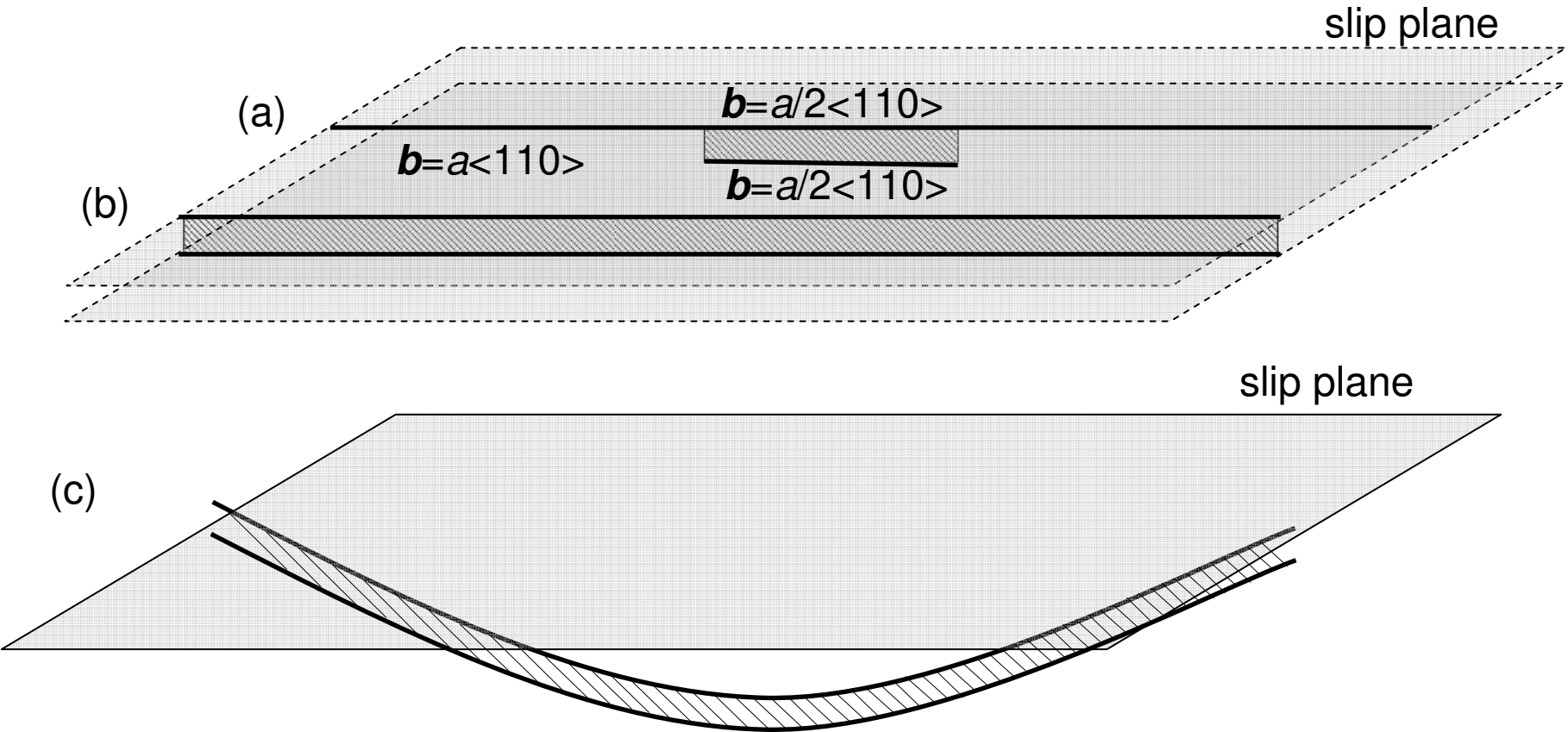


Fig.11

